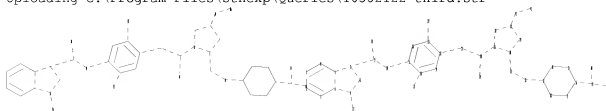


=>

Uploading C:\Program Files\Stnexp\Queries\10562122-third.str



chain nodes :

11 12 13 14 21 22 23 24 25 31 32 39 40 41 42 43

ring nodes :

1 2 3 4 5 6 7 8 9 15 16 17 18 19 20 26 27 28 29 30 33 34 35
36 37 38

chain bonds :

7-12 9-11 12-13 12-14 14-15 17-22 18-23 20-21 23-24 24-25 24-26 28-42
30-31 31-32 32-33 36-39 39-40 39-41 42-43

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 15-16 15-20 16-17 17-18 18-19
19-20 26-27 26-30 27-28 28-29 29-30 33-34 33-38 34-35 35-36 36-37 37-38

exact/norm bonds :

5-6 5-7 6-9 7-8 7-12 8-9 9-11 12-13 12-14 14-15 17-22 18-23 20-21 23-24
24-25 24-26 26-27 26-30 27-28 28-29 28-42 29-30 30-31 31-32 32-33 33-34
33-38 34-35

35-36 36-37 36-39 37-38 39-40 39-41 42-43

normalized bonds :

1-2 1-6 2-3 3-4 4-5 15-16 15-20 16-17 17-18 18-19 19-20

isolated ring systems :

containing 1 : 15 : 26 : 33 :

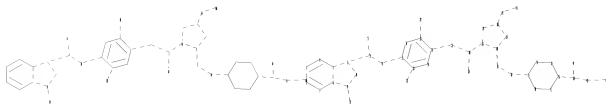
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:CLASS 22:CLASS
23:CLASS 24:CLASS 25:CLASS 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS
32:CLASS
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:CLASS 40:CLASS 41:CLASS
42:CLASS 43:CLASS

L1 STRUCTURE UPLOADED

=>

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```

chain nodes :
11 12 13 14 21 22 23 24 25 31 32 39 40 41 42 43 44
ring nodes :
1 2 3 4 5 6 7 8 9 15 16 17 18 19 20 26 27 28 29 30 33 34 35
36 37 38
chain bonds :
7-12 9-11 12-13 12-14 14-15 17-22 18-23 20-21 23-24 24-25 24-26 28-42
30-31 31-32 32-33 36-39 39-40 39-41 41-44 42-43
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 15-16 15-20 16-17 17-18 18-19
19-20 26-27 26-30 27-28 28-29 29-30 33-34 33-38 34-35 35-36 36-37 37-38
exact/norm bonds :
5-6 5-7 6-9 7-8 7-12 8-9 9-11 12-13 12-14 14-15 17-22 18-23 20-21 23-24
24-25 24-26 26-27 26-30 27-28 28-29 28-42 29-30 30-31 31-32 32-33 33-34
33-38 34-35
35-36 36-37 36-39 37-38 39-40 39-41 41-44 42-43
normalized bonds :
1-2 1-6 2-3 3-4 4-5 15-16 15-20 16-17 17-18 18-19 19-20
isolated ring systems :
containing 1 : 15 : 26 : 33 :

```

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Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:CLASS 22:CLASS
23:CLASS 24:CLASS 25:CLASS 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS
32:CLASS
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:CLASS 40:CLASS 41:CLASS
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44:CLASS

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L3 STRUCTURE UPLOADED

=> d his

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FILE 'REGISTRY' ENTERED AT 07:24:17 ON 18 APR 2008

L1 STRUCTURE UPLOADED

L2 7 S L1 SSS FULL

FILE 'STNGUIDE' ENTERED AT 07:25:03 ON 18 APR 2008

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L3 STRUCTURE UPLOADED
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L5 3 S L2 NOT L4

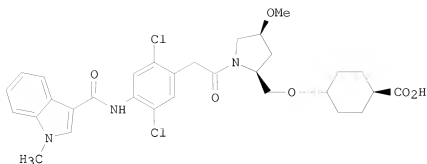
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L6 5 S L5
L7 1 S US200!-562122/APPS
L8 1 S L6 AND L7
L9 4 S L6 NOT L7

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L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:99497 CAPLUS <<LOGINID:20080418>>
DN 142:197874
TI Preparation of indole derivative containing cyclohexanecarboxylic acid
moiety as VLA-4 inhibitors
IN Ono, Makoto; Noguchi, Shigeru
PA Daiichi Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 19 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|------------------|--------------|
| PI | WO 2005009992 | A1 | 20050203 | WO 2004-JP10457 | 20040723 |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| | RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| | CA 2528586 | A1 | 20050203 | CA 2004-2528586 | 20040723 |
| | EP 1650205 | A1 | 20060426 | EP 2004-747846 | 20040723 |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK | | | | |
| | CN 1826336 | A | 20060830 | CN 2004-80021230 | 20040723 |
| | US 20070105936 | A1 | 20070510 | US 2005-562122 | 20051223 <-- |
| | MX 2006PA00850 | A | 20060330 | MX 2006-PA850 | 20060123 |
| PRAI | JP 2003-201062 | A | 20030724 | | |
| | WO 2004-JP10457 | W | 20040723 | | |
| OS | CASREACT 142:197874 | | | | |
| GI | | | | | |



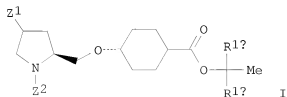
AB A VLA-4 (very late antigen-4) inhibitory compound I sodium salt pentahydrate having high solubility in water and long-term stability was prepared. Thus, EDCI-mediated acylation of trans-4-[(4S)-methoxy-(2S)-pyrrolidinylmethoxy]cyclohexanecarboxylic acid Me ester with [2,5-dichloro-4-[(1-methyl-1H-3-indolylcarbonyl)amino]phenyl]acetic acid, followed by treatment with aqueous NaOH afforded compound I sodium salt pentahydrate. Compound I sodium salt pentahydrate is claimed useful for the treatment of inflammation, diabetes, etc.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d 19 tot bib abs hitstr

L9 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2007:352105 CAPLUS <<LOGINID::20080418>>
DN 146:379822
TI Stereoselective preparation of trans-cyclohexanes as intermediates for
VLA-4 inhibitors
IN Chiba, Atsushi
PA Daiichi Seiyaku Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 61pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|-------------------|------|----------|-----------------|----------|
| PI | JP 2007077032 | A | 20070329 | JP 2005-263466 | 20050912 |
| PRAI | JP 2005-263466 | | 20050912 | | |
| OS | MARPAT 146:379822 | | | | |
| GI | | | | | |



AB Title compds. I [Z1 = β -OR₆; Z2 = H; R1a, R1b = lower alkyl,

(un)substituted Ph, (un)substituted PhCH₂; R₆ = lower alkyl] are prepared by esterification of trans-4-HOZ3CO₂MeR_{1a}R_{1b} (Z₃ = cyclohexanediyl; R_{1a}, R_{1b} = same as above) with (S)-(+)-epihalohydrin, treatment with H₂C:CHX₃ (X₃ = MgCl, MgBr, MgI, Li), Mitsunobu reaction with [(un)substituted benzo]succinimide, treatment with hydrazines, amidation with (un)substituted benzoyl compds., cyclization in the presence of iodine, and via I [Z₁ = α-R₃CO₂; Z₂ = H; R_{1a}, R_{1b} = same as above; R₃ = (un)substituted Ph], I [Z₂ = R₄O₂C; R₄ = (un)substituted PhCH₂, Ph₂CH; Z₁, R₃, R_{1a}, R_{1b} = same as above], I [Z₁ = α-OH; Z₂, R₄, R_{1a}, R_{1b} = same as above], I [Z₁ = β-R₅CO₂; R₅ = H, lower alkyl, (un)substituted Ph; Z₂, R₄, R_{1a}, R_{1b} = same as above], and I [Z₁ = β-OH; Z₂, R₄, R_{1a}, R_{1b} = same as above]. Thus, I (Z₁ = α-OH, Z₂ = cbz, R_{1a}, R_{1b} = Me) was formylated, hydrolyzed, treated with MeI, and deprotected to give I (Z₁ = β-MeO, Z₂ = H, R_{1a}, R_{1b} = same as above), which was amidated with 2,5-dichloro-4-[(1-methylindol-3-yl)carboxamido]phenylacetic acid to afford the corresponding amide.

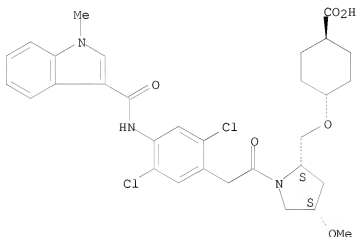
IT 793669-59-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of VLA-4 inhibitors from trans-cyclohexanecarboxylic acid tertiary alc. esters)

RN 793669-59-7 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[{(2S,4S)-1-[2-[2,5-dichloro-4-[(1-methyl-1H-indol-3-yl)carbonyl]amino]phenyl]acetyl]-4-methoxy-2-pyrrolidinyl]methoxy]-, trans- (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2005:638842 CAPLUS <<LOGINID::20080418>>

DN 143:153280

TI Process for preparation of pyrrolidine derivatives

IN Takayanagi, Yoshihiro; Yamada, Toshihide; Furuya, Yukito; Yoneda, Yoshiyuki

PA Daiichi Pharmaceutical Co., Ltd., Japan

SO PCT Int. Appl., 76 pp.

CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO.

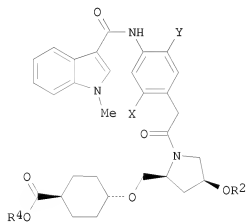
KIND

DATE

APPLICATION NO.

DATE

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| | W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GE, GH, GM, GR, GU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | |
| | RW: | BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | |
| | EP 1698621 | A1 | 20060906 | EP 2004-807936 | 20041227 |
| | R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS | | | |
| | US 20070149607 | A1 | 20070628 | US 2006-584141 | 20060626 |
| PRAI | JP 2003-431686 | A | 20031226 | | |
| | WO 2004-JP19581 | W | 20041227 | | |
| OS | MARPAT 143:153280 | | | | |
| GI | | | | | |



I

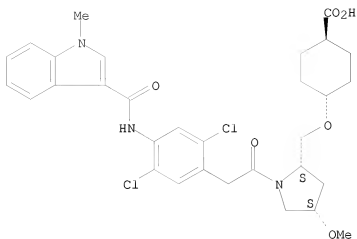
AB Disclosed is an advantageous method for producing an intermediate compound I [wherein X = H or halo; Y = halo or alkoxy; R₂ = alkyl; R₄ = (un)substituted alkyl or aralkyl], which is useful for obtaining a safe compound having excellent VLA-4 inhibitory activity. For example, the compound I•Na (X = Y = Cl; R₂ = Me; R₄ = H) was prepared in a multi-step synthesis.

IT 858362-36-4P
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; preparation of pyrrolidine derivs.)

RN 858362-36-4 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[[2S,4S)-1-[2-[2,5-dichloro-4-[[[1-methyl-1H-indol-3-yl]carbonyl]amino]phenyl]acetyl]-4-methoxy-2-pyrrolidinyl]methoxy]-, sodium salt (1:1), trans- (CA INDEX NAME)

Absolute stereochemistry.



● Na

IT 835901-02-5P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

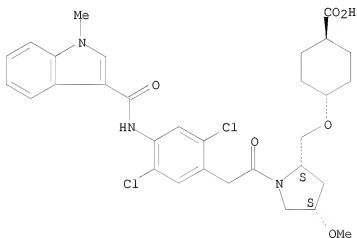
(preparation of pyrrolidine derivs.)

RN 835901-02-5 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[[(2S,4S)-1-[[[2,5-dichloro-4-[(1-methyl-1H-indol-3-yl)carbonyl]amino]phenyl]acetyl]-4-methoxy-2-pyrrolidinyl]methoxy]-, monosodium salt, pentahydrate, trans- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



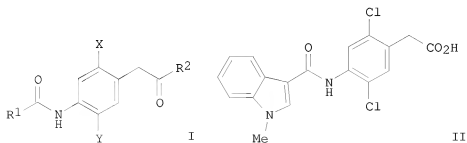
● Na

● 5 H₂O

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:612230 CAPLUS <<LOGINID::20080418>>
DN 143:133271
TI Process for preparation of phenylacetic acid derivatives
IN Nakayama, Atsushi; Noguchi, Shigeru; Furuya, Yukito; Okano, Katsuhiko
PA Daiichi Pharmaceutical Co., Ltd, Japan
SO PCT Int. Appl., 68 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|-------------------|--|----------|-----------------|----------|
| PI | WO 2005063678 | A1 | 20050714 | WO 2004-JP19578 | 20041227 |
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| | RW: | BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | |
| | EP 1698611 | A1 | 20060906 | EP 2004-807933 | 20041227 |
| | R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS | | | |
| | US 20070149606 | A1 | 20070628 | US 2006-584240 | 20060626 |
| PRAI | JP 2003-431680 | A | 20031226 | | |
| | JP 2004-283082 | A | 20040929 | | |
| | JP 2004-312335 | A | 20041027 | | |
| | WO 2004-JP19578 | W | 20041227 | | |
| OS | MARPAT 143:133271 | | | | |
| GI | | | | | |



AB This invention pertains to a method for producing heterocycle substituted phenylacetic acid derivs. I [wherein R1 = (un)substituted aryl or heteroaryl; R2 = (un)substituted alkoxy, aralkyloxy, phenoxy, etc.; X = H or halo; Y = halo or alkoxy]. For example, the compound II was prepared in a multi-step synthesis. This invention provides a convenient method to prepare phenylacetic acid derivs. which are useful intermediates for the preparation of medicinal compds.

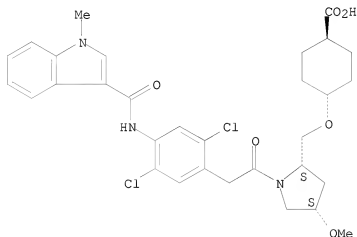
IT 858362-36-4P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; preparation of phenylacetic acid derivs.)

RN 858362-36-4 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[[(2S,4S)-1-[2-[2,5-dichloro-4-[[[(1-methyl-1H-indol-3-yl)carbonyl]amino]phenyl]acetyl]-4-methoxy-2-pyrrolidinyl]methoxy]-, sodium salt (1:1), trans- (CA INDEX NAME)

Absolute stereochemistry.



● Na

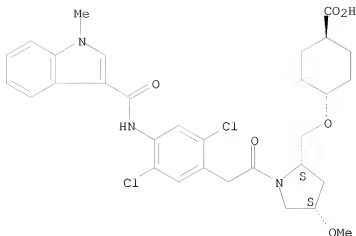
IT 835901-02-5P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation) (preparation of phenylacetic acid derivs.)

RN 835901-02-5 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[[(2S,4S)-1-[2-[2,5-dichloro-4-[[[(1-methyl-1H-indol-3-yl)carbonyl]amino]phenyl]acetyl]-4-methoxy-2-pyrrolidinyl]methoxy]-, monosodium salt, pentahydrate, trans- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Na

● 5 H₂O

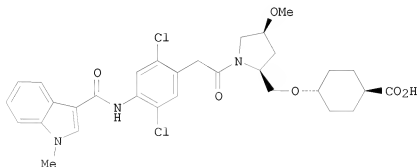
RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on SIN
AN 2004:996121 CAPLUS <<LOGINID::20080418>>
DN 141:410814
TI Process for preparation of pyrrolidine derivatives
IN Nakayama, Atsushi; Machinaga, Nobuo; Yoneda, Yoshiyuki; Setoguchi, Masaki
PA Daiichi Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|--|----------|-----------------|----------|
| WO 2004099136 | A1 | 20041118 | WO 2004-JP6471 | 20040507 |
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| RW: | BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, | | | |

SN, TD, TG

| | | | | |
|--|----|----------|----------------|----------|
| EP 1623975 | A1 | 20060208 | EP 2004-731729 | 20040507 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, | | | | |
| IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK | | | | |
| US 20070105935 | A1 | 20070510 | US 2005-556043 | 20051108 |
| US 7345179 | B2 | 20080318 | | |
| PRAI JP 2003-131978 | A | 20030509 | | |
| JP 2003-144430 | A | 20030522 | | |
| JP 2003-209579 | A | 20030829 | | |
| WO 2004-JP6471 | W | 20040507 | | |
| OS MARPAT 141:410814 | | | | |
| GI | | | | |



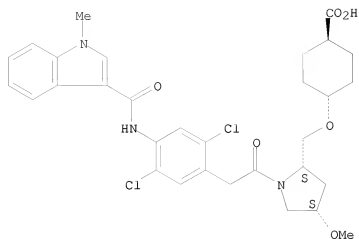
AB This invention pertains to a method for industrially advantageously producing 1,4-trans-cyclohexanecarboxylic acid derivative I which comprises reduction and isomerization processes. Trans-4-[(4S)-Methoxy-(2S)-pyrrolidinylmethoxy]cyclohexanecarboxylic acid Et ester (preparation given) was reacted with 2,5-dichloro-4-[(1-methyl-1H-indol-3-yl)carboxamido]phenylacetic acid (preparation given) to give I Et ester (99.8%).

IT 793669-59-7P
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (preparation of pyrrolidine derivs.)

RN 793669-59-7 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[[(2S,4S)-1-[2-[2,5-dichloro-4-[[[(1-methyl-1H-indol-3-yl)carbonyl]amino]phenyl]acetyl]-4-methoxy-2-pyrrolidinyl]methoxy]-, trans- (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT